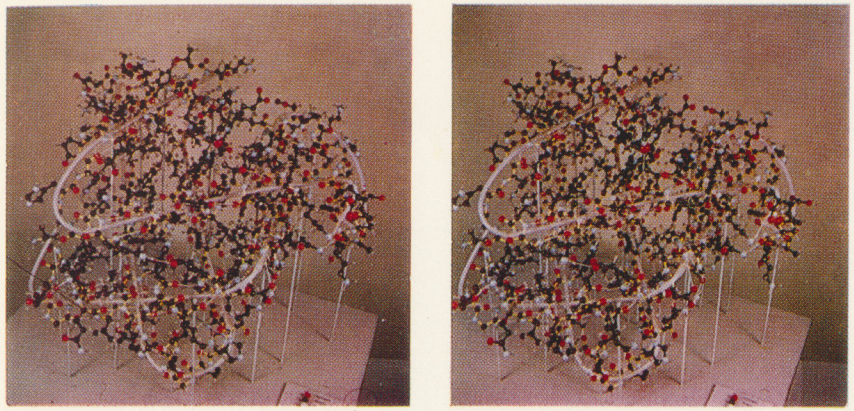

Frontispiece. Stereo-photograph of a model of the myoglobin molecule

The white rod follows the course of the polypeptide chain. Atoms are represented by coloured spheres (carbon, black; nitrogen, blue; oxygen, red; sulphur, green; hydrogen, dull grey). The larger sphere near the centre of the molecule represents the haem iron. Main-chain covalent bonds are coloured yellow, side-chain ones black, and hydrogen bonds are indicated by thin white nylon rods. The amino end of the molecule is at the bottom left of the field of view and the terminal carboxyl group at the top left.

PROGRESS IN STEREOCHEMISTRY

4

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THE USE OF MODELS IN STEREOCHEMISTRY

Anne Walton

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1 INTRODUCTION

Models illustrating stereochemical principles have been in use for over 100 years. Pasteur (1848), Dewar (1867), Le Bel (1874), van't Hoff (1874) and Kelvin (1889) were among the first to appreciate their potentialities. During the last few decades, interest in molecular and crystal-structure models has increased considerably, and research laboratories and teaching institutions at all levels use them extensively as aids to understanding the spatial relationships between atoms and ions.

As has been stressed by Mislow (1965), it must be accepted that any model can convey only partial truth concerning a particular system:

it may display admirably some stereochemical aspects of a molecular situation and be positively misleading about others. The perfect model simply does not exist.

Several types of model are now commercially available, and the literature contains a number of recent references to a variety of home-made ones. This Chapter is intended to be a practical guide to those who wish to know the scope and limitations of models which can be bought or made at the present time. The main criteria used in assessing the utility of the different types are their precision, the ease with which they can be assembled or taken apart, their mechanical strength, the number and range of components and the cost. While some model types are of fairly general application, others have been designed for specific purposes, and this is indicated where appropriate. Discussion is largely limited to models of the 'static' type of which there are three main kinds: (*a*) space-filling, in which the shapes representing atoms are in contact or very nearly so; (*b*) ball and spoke, in which spheres representing atoms or ions are separated from each other by rods or tubes; and (*c*) skeletal, in which only the molecular framework is indicated. The division between these is somewhat arbitrary, and some intermediate types exist. 'Dynamic' models in which atomic and molecular motion is simulated are not dealt with in detail, nor are constructional devices, although some reference to these is made in Section 5. No attempt has been made to describe all possible variants of a particular type, but representatives of each have been selected for detailed treatment.

There are two main descriptive Sections. The first deals with models of which all components are commercially available, often as sets of varying complexity. The second covers a number of miscellaneous types; some components can be bought, but information for the 'Do-it-yourself' enthusiast is also given.

Very few references before 1960 had to be included, since an excellent bibliography (Smith, 1960) on molecular and crystal-structure models, published by the U.S. National Bureau of Standards, covers the literature up to and including 1959. Moreover, there have been several new developments in the last few years which, it is hoped, will be of greater interest to potential users of models than an historical survey. On the whole, reference has been confined to generally useful applications and new developments rather than to standard models used to illustrate a specific point.

Manufactured models representing atoms of a particular element are usually coloured according to one of the colour conventions in common use. Most British manufacturers conform to the recommendations of the x-ray Analysis Group of the Institute of Physics (1947). This colour code is given in TABLE 1 together with the colours of the atom models which are to be discussed.

TABLE 1. COLOURS OF ELEMENTS USED IN MOLECULAR AND CRYSTAL-STRUCTURE ATOM MODELS

Trade name or manufacturer	C	H	O	N	F	Cl	Br	I	S	P	Si	*Metals*
Catalin covalent	black	cream	red	blue	pale green			dark green	dark red	blue	grey	yellow or violet
Catalin ionic	black	white	red	blue	pale green	deepening shades of green		dark green	dark red	dark blue	grey	various
Courtauld	black	cream	red	blue	light green	grass green	blue-green	dark green	yellow	purple	grey	silver or copper
C.P.K.	black	white	red	blue	pale green	green	brown	violet	yellow	pale yellow	—	silver
Crystal Structures Ltd.	black	white	red	blue	yellowish green	light green	mid-green	dark green	yellow	purple	black or grey	silver, gold, copper, bronze
Dreiding	black	—	red	blue	beige	green-yellow	red-brown	dark brown	yellow	violet	silver	various
F.M.M.	black	white	red	blue	light green	dark-green	orange	brown	dark yellow	violet	light yellow	grey
Gallenkamp	black	white	red	blue	one halogen model—green				yellow	—	—	brown
Godfrey space-filling	black	white	red	blue	—	green	—	—	yellow	—	—	white
Leybold molecular	black	white	red	blue	dark yellow	green	brown	violet	yellow	light-brown	light grey	silver or bronze
S.A.S.M.	black	red	light blue	dark blue	straw yellow	light green	dark brown	violet	yellow	grey-brown	light grey	silver or orange
Institute of Physics	black	cream or white	red	blue	yellowish green	light green	mid-green	dark green	yellow	purple	black or grey	brown, silver or gold

2 SPACE-FILLING MODELS

This type of model corresponds more closely than any other to a scaled-up molecule. The outer surface represents the van der Waals's envelope and thus defines the closest approach of another molecule or atom whether contact is transitory, as in gas-phase collisions, or relatively static, as in crystals. In general, the atom models are derived from spheres which have radii proportional to the van der Waals's ones. Perpendicular to each bond direction, a segment of the sphere is removed leaving a plane face. The distance from the centre of this face to that of the sphere is proportional to the covalent radius of the bonded atom. Since this radius may vary widely according to environment, a number of different atom models of the same element are necessary for accurate representations, particularly when multiple bonding is possible or when the atom can form part of a ring system. Many atom models appear to bear little relationship to the sphere from which they were derived. An aliphatic carbon atom, for example, may look like a tetrahedron and an aromatic ring carbon like a trigonal prism. Furthermore, in order to permit slight distortion and to prevent a spurious steric hindrance effect, some atom models have been truncated at the points of intersection of the plane faces. The values for the covalent and van der Waals's radii used in the construction of models are generally those of Pauling (1960) or those quoted in the Chemical Society Special Publications No. 11 and 18 (Sutton, 1958 and 1965). On the whole, manufacturers of the more precise models appear to have made every effort to keep abreast of current developments and to use up-to-date and reliable data.

This is true also of bond angles. Most atom models are constructed with those which commonly occur, but the same problem arises as with the radii in that variations from the 'ideal' angle can be quite considerable in different compounds. The best precision models allow for this by providing distortable links which can, in some cases, be locked in the distorted position. In this way, variation in angle up to about 12° is possible.

A further difficulty is that of free or restricted rotation about bonds. The snap-fastener link described below is one kind which permits free rotation, and there are techniques such as using double links which prevent rotation completely, while others allow it within limits.

One of the great advantages of the space-filling models is that they are able to illustrate, and predict, steric hindrance. Quite accurate measurements can be made using the precision models. For teaching purposes, they can be used to demonstrate many structural principles such as structural isomerism, various steric effects, different conformations, strained structures and some reaction mechanisms. Certain of these models have been designed particularly for the biochemist. The new, light plastic hollow models with strong but distortable links are

TABLE 2. SPACE-FILLING ATOM MODELS

Manufacturers	Catalin	Courtauld	C.P.K.	Godfrey	Leybold
Total number of species available	53	34	24	26	45
No. of elements represented	16	13	12	16	17
No. of different species:					
carbon	13	8	7	3	12
oxygen	8	5	3	3	5
nitrogen	8	8	4	3	10
metals	5	2	2	4	5
Scale	1 Å ≡ 1 cm	1 Å ≡ 0·8 in ≡ 2·03 cm	1 Å ≡ 1·25 cm	1 Å ≡ 1·65 cm	1 Å ≡ 1·5 cm
Precision	good	very good	very good	fair	good
Material, colouring, identification	solid, self-coloured cast resin; rather dense material (see TABLE 3)	hollow models of self-coloured light polystyrene; identity code embossed	hollow models, labelled, of self-coloured light plastic	hollow, flexible models of self-coloured P.V.C.	painted wooden models; different species of same element distinguished by colour on some faces
Type of structure which can be assembled (some examples)	organic and organometallic, organo-boron compounds, metal complexes, silicates	biochemical structures, many organic and inorganic compounds, metal complexes, organometallic compounds, silicates	biochemical structures, some simple compounds, metal complexes	chiefly organic, some relatively simple inorganic, compounds	biochemical structures, organic compounds, metal chelates, polymers
Atom models or groups (selected examples)	block rings (benzene and naphthalene); distorted benzene block for fused ring systems	block rings; special H-bond model	twin carbon atom models for those common to two rings; special H-bond model	—	small rings and several groups, e.g. $-NO_2$, as single units; twin atoms for condensed rings; special H bond; pre-assembled groups for DNA construction
Special features	free and restricted rotation; mechanism for fused rings; 3- and 4-membered rings possible; long links for 'exploded' models. Stuart type with 20 per cent reduction in van der Waals's radius	free and restricted rotation; mechanism for fused rings; small rings possible; large atom models chamfered; nylon rods for extra rigidity (see TABLE 3)	free and restricted rotation; mechanism for fused rings; preassembled structures available (see TABLE 3)	compressible; stability enhanced, rotation prevented by metal staples	free and restricted rotation; mechanism for fused rings; pre-assembled units; Stuart-type models (see TABLE 3)

TABLE 3. CONNECTORS USED IN SPACE-FILLING MODELS

Manufacturers	Catalin	Courtauld	C.P.K.	Godfrey	Leybold
Description	hard, tubular rubber pegs; 10 cm steel connecting pins for exploded models	brass standard link 0·4 in long; press-stud mechanism; rubber collar fitted over link; bent links for small rings and adjustable link	several types; made of Texin (hard, rubber-like, resilient and flexible); colour-coded	flat pieces of polythene in 4 different lengths, barbed at one or both ends; staples to strengthen assembly; magnets for H bonds	metal press studs; hook and eye H-bond mechanism
Variation in length	only by partial insertion of peg in socket which weakens link	adjustable link with screw thread allows ±0·1 Å	short link 0·05 Å less than standard link, long link 0·08 Å greater; adjustable H-bond link	only by partial insertion of connector into atom model	none
Variation in angle	~5°; linked models not quite touching	rubber collar only, 12°; with yellow plastic ring, 6°; with red plastic ring, 0°	up to ±8°	whole assembly very flexible	very slight, as models are virtually in contact
Strength of assembled link	quite good for small assemblies; large should be wired	good even for very large assemblies: very strong linking mechanism; light model atoms	good even for very large assemblies; strong linking mechanism; light model atoms	stability of assembly improved by staples	good even for very large assemblies; strong linking mechanism; little friction in link—groups tend to rotate when assembly moved
Mechanism for restricting rotation	metal pin and socket on either side of connector socket for locking multiple-bonded atom models in position	nylon rods inserted into sockets prevent rotation about single bonds; double connector sockets for multiple bonds	special links with projections fitting into notches in connector sockets restrict rotation; 'gluing' connectors for permanent non-rotating links	can be prevented by stapling	prevented by metal clamping spring inserted into slits on multiple-bonded atom models
Ease of assembly and separation	pliers supplied for insertion and removal of pegs; assembly rapid	insertion and extraction magazine supplied: quick and easy manipulation of connectors; atom models can be pulled apart manually if mutually inclined	construction tool supplied for assembly and dismantling	assembly requires practice, dismantling very easy	easy to assemble: pressed together manually; separator tool supplied to lever them apart (also to remove connectors)

well suited to the construction of naturally-occurring macromolecules. For these, strength and rigidity are essential but, at the same time, some degree of distortion must be possible. Much of the literature on space-filling models supplied by the manufacturers deals almost exclusively with organic structures. Inorganic chemists should not, however, be deterred, as many of these can be used for building co-ordination compounds and quite a large range of organometallic structures.

Models which are used to demonstrate the close packing of spheres and similar phenomena are also space-filling, but since they are essentially ionic structures they are discussed along with other ionic models in the next Section.

Five examples of space-filling models which include some of the best-known types have been selected for more detailed discussion. As far as possible, data have been tabulated to facilitate comparison (TABLES 2 and 3).

A. *Catalin Covalent Models*

These are essentially Stuart models designed by the National Chemical Laboratory. The range of available ones is large, and a great variety of structures can be assembled. Inorganic chemists may find them more

FIGURE 8.1 (continued overleaf)

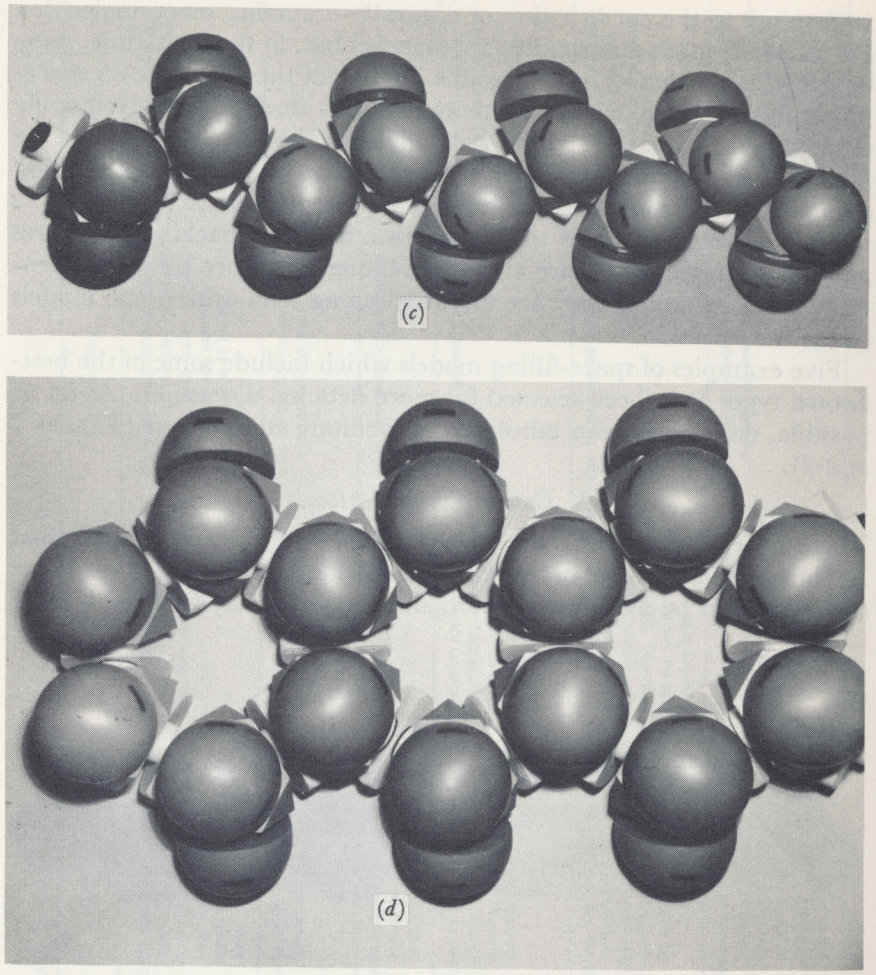


FIGURE 8.1. Space-filling models of silicate chains: (*a*) Catalin* pyroxene; (*b*) Catalin* amphibole; (*c*) Courtauld** pyroxene; (*d*) Courtauld** amphibole

* Supplied on loan by manufacturers
** Reproduced by permission of Dr. W. French, Queen Mary College, University of London and Mr. D. Taylor of Griffin & George Ltd.

suited to their requirements than other space-filling models, particularly if used in conjunction with the Catalin ionic models as suggested by the manufacturers. Five different metal models are made, and there is also an oxygen-atom model with a 140° bond angle with which silicate structures can be assembled (FIGURE 8.1*a* and *b*). The stability of models of large molecules can be improved by passing wire through the whole assembly. The original Stuart models (Stuart, 1934) had the full van der Waals's radii and the plane faces were in contact, thus preventing any distortion. The Catalin models have the van der Waals's

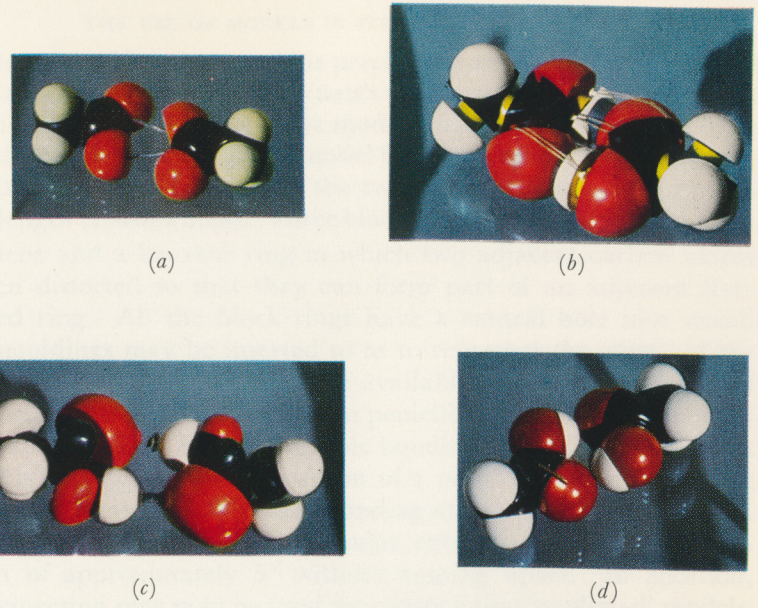


FIGURE 8.2. Space-filling models of the acetic acid dimer molecule: (*a*) Catalin Covalent; (*b*) Courtauld; (*c*) Godfrey; (*d*) Leybold

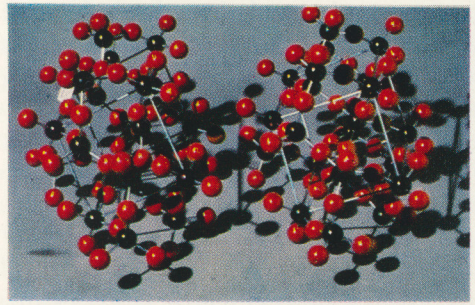


FIGURE 8.3. Pre-assembled ball and spoke models (Crystal Structures Ltd.): α- and β-quartz

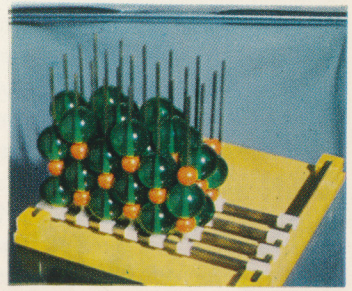


FIGURE 8.4. Sodium chloride crystal structure built on Catalin adjustable base

radii reduced by 20 per cent. This precludes spurious steric hindrance but may also reduce the van der Waals's envelope to such an extent that steric hindrance is not shown in the model when it is known to occur in the molecule. There is no special model for a hydrogen bond, and it can be simulated only by connecting the two donor atoms with wire of a suitable length (FIGURE 8.2*a*). Three block rings are available: benzene, naphthalene and a benzene ring in which two adjacent carbon atoms have been distorted so that they can form part of an adjacent five-membered ring. All the block rings have a central hole into which rubber mouldings may be inserted so as to represent the extent of the π-orbitals. Special carbon atoms are available for the construction of fused 4- and 5-membered rings (as in penicillin); 3- and 4-membered rings are also possible. Where multiple bonding occurs, rotation about the bond is prevented by the insertion of a metal pin on the bonding face of one atom model into a corresponding socket on the adjacent one. The models are joined by short tubular rubber pegs which allow a distortion of approximately 5° without coming apart. In addition, 10 cm connecting pins may be used for constructing 'exploded' models.

B. *Courtauld models*

These precision models were developed by Courtaulds Ltd. (Robinson, 1966). They have several advantages over the original Stuart models. First of all, the whole of the covalent radius does not reside in the atom model itself but partly in the link which is 0·4 in long. This permits distortion of the link and allows the user to see much more clearly the spatial relationships between the atoms. Both these features are particularly desirable in the construction of macromolecules. The distortable link enables the full van der Waals's radii to be used for most atom models, thus ensuring an accurate representation of the van der Waals's envelope. Secondly, techniques have been devised which limit angular distortion to fixed values. Each link is fitted with a soft rubber collar which permits a distortion of 12° when strained but when unstrained holds the atom faces perpendicular to the connecting link. If a yellow plastic ring is fitted over the rubber collar, angular distortion is restricted to 6°. If a red one is used instead, virtually no angular distortion is possible. In all these cases, rotation about single bonds can occur but the friction is sufficient for configurations to be retained when the model is moved. The links fit into press-stud sockets with strong springs; a magazine is provided which greatly facilitates their insertion and extraction. It is quite easy to separate linked atoms manually if they are inclined at an angle to one another. An adjustable link with a screw thread can be used to vary bond lengths by $\pm 0{\cdot}1$ Å. Multiple-bonded atoms have double sockets to prevent rotation, but in situations where this is known not to occur about single bonds, nylon rods may be

inserted in sockets on opposing atoms. Very slight distortion is still possible because of the flexibility of the rods. The nylon rods can also be used to lock atoms (e.g. tetrahedral carbon atoms) in a particular conformation. Bent links are used in the construction of 3- and 4-membered rings. This technique is mechanically desirable, and some theoretical justification may also be claimed for it (Coulson and Moffitt, 1949; Robinson, 1966).

The new Courtauld model atoms are hollow and made of light plastic with the colour incorporated into it. Each model is identified by an embossed code mark, and to obviate ambiguity particular model faces are distinguished. The benzene carbon model, for example, has one face with a double socket and two with single sockets. One of the latter is used in ring construction, while the other is engraved to indicate that it represents the single bond face. The alternating single and double sockets in the benzene ring enable canonical forms to be represented.

The new plastic models can be combined with the old wooden ones, but it is recommended that the new links be used. There may be some loss of accuracy owing to slight differences in dimension, since the new models conform as far as possible to revised data published in the literature. The new hydrogen atom model has a van der Waals's radius proportional to 1·0 Å, although Pauling's value is 1·2 Å (Pauling, 1960). It is claimed (Robinson, 1966) that this compromise value is justified, since many molecular models could not have been constructed using the larger value: severe steric hindrance was implied in situations where it was known not to occur to any great extent. A similar compromise has been effected with the chlorine, bromine and iodine models. These have been chamfered at the bond faces to enable carbon tetrahalides and hexahaloaromatic models to be constructed. This does, however, result in there being no bond-angle distortion in *ortho*-substituted aromatic models, although this is observed in the molecules themselves.

Several special models have been designed for use in different ring systems. In particular, there is a new nitrogen model with planar bonds for use in 5-membered rings such as occur in nucleotides.

A cylindrical model representing the hydrogen bond has been designed. It has a radius corresponding to 0·5 Å, and the plane face is joined by the usual linking mechanism to one of the donor atoms. The other face has a circular groove into which is inserted a vulcanized fibre strip. This rests on the 'hydrogen-bonding' surface of the other donor atom and can be attached to it by elastic bands. The carbonyl–oxygen model is a sphere with a segment removed, and in order to prevent the hydrogen-bond model sliding off the rounded surface, the planar face of the oxygen model has three pegs to which elastic bands may be attached. These then pass over the model and are attached to three similar ones on the plane surface of the hydrogen-bond model

(FIGURE 8.2*b*). Although objections may be raised to the use of elastic bands on aesthetic grounds, they do seem to function quite satisfactorily. The fibre strip is not used for representations of non-linear hydrogen bonds.

Co-ordination complexes are constructed using the metal-atom model for octahedral or square planar co-ordination. The covalent radius of 1·25 Å can be varied by ±0·1 Å by use of the adjustable link. The copper atom model (radius, 1·35 Å) is designed for tetrahedral complexes, but where smaller radii for the central atom are required, the silicon (radius, 1·17 Å) or sulphur (1·0 Å) models can be used. Again, the adjustable link serves to vary bond lengths as necessary. A co-ordination oxygen model has been designed for aquo-complexes, and a silicate oxygen with a 141° angle enables regular silicate structures to be assembled (FIGURE 8.1*c* and *d*).

C. *C.P.K. Models*

These are modifications of the Corey–Pauling models (Corey and Pauling, 1953) with new connectors designed by Koltun (1965). The abbreviation C.P.K. is now generally used instead of the rather lengthy Corey–Pauling–Koltun. Federal U.S. agencies, such as the National Institutes of Health and the National Science Foundation, have supported the development of these models, together with the American Society of Biological Chemists. Like the Courtauld ones, these are precision models, and it is claimed that the bond angles are accurate within ±0° 30′, the covalent radii ±0·01 Å and van der Waals's radii ±0·03 Å. The atom models are hollow, and made of light, strong self-coloured plastic. Many of the principles used in the design of Courtauld models have been incorporated into the C.P.K. models. The atom models are smaller, the scale being 1·25 cm ≡ 1 Å against 2 cm ≃ 1 Å for Courtauld models, but otherwise their appearance is very similar. The spheres are labelled, and where there may be ambiguity, the covalent radius is stamped on the appropriate face. The hydrogen model, unlike the others, is elastically compressible and has a permanent connector link. A carbon-atom pair is available which represents the two carbon atoms common to a fused 6- and 5-membered ring system such as occurs, for example, in tryptophan. The larger halogen atoms are chamfered in the same way as the Courtauld models. There are no special species available for 3- and 4-membered rings. Tetrahedral nitrogen can be converted into amine nitrogen by use of an 'amine cap' which is attached by a short hollow connector link to the nitrogen; the cap is pierced so as to be able to form a hydrogen bond. The model used for linear hydrogen bonds has the usual connector link on one face and a barbed shank on the other, which is inserted into one of three slots on the rounded surface of the carbonyl–oxygen models. The barbs

are arranged in sets so that, depending on which set is used, the hydrogen-bond length may be adjusted. A version of the linear H bond with a 'hook and eye' mechanism is now also available. The two oxygen models used to demonstrate hydrogen bonding have 3 parallel slots on their rounded surfaces. Thus the angle of insertion of the shank from the hydrogen bond model may be varied. A special non-linear hydrogen bond model is in process of development and expected to be on the market before long. Where multiple bonding is possible, the sockets of the atom models have notches into which projections on the connectors can fit, thus locking the linked atoms in position and preventing rotation about the link. The tetrahedral carbon atom has 3 notches in the sockets so that the three-fold rotational potential may be demonstrated.

The main difference between the C.P.K. and Courtauld models is the linking mechanism. The link is strong in both types and contributes to the interatomic distance, so that the atoms are not in contact, giving a high degree of 'transparency' to the assembled models. Moreover, the friction is sufficient for side chains to retain the correct orientation.

The C.P.K. connectors are made of a hard rubber-like elastomer (Texin) which is both resilient and flexible. There are several different types, all colour-coded. The standard link gives the normal bond length for a particular atom; its colour is off-white. The short link is blue and shortens the bond by 0·05 Å, while the long one is red and lengthens it by 0·08 Å. In addition, there is a locking link with splines (projections), coloured grey, which is used to prevent rotation, and a special locking link for carbon atoms (black) which is the standard length but can be locked in different positions as the link is rotated. A further one is also provided which can be glued in position for making permanent connections. Finally, a standard-length link has been designed which can be inserted into special atom models made by the user, providing these have a suitable C.P.K. socket. A construction tool is used in assembly and taking apart. The link is placed in a 'well' on the tool and pressed into an atom-model socket. The second atom is then pressed on with a slight twist. The other end of the construction tool has a forked end and a levering blade. The former is used to remove links and the latter to separate atoms. The connectors allow bond angles to vary up to $\pm 8°$.

The C.P.K. models have been designed primarily for the construction of proteins and nucleic acids, but they can be used to construct many smaller organic molecules and some metal complexes.

Two metal-atom models are available, one covalent and one ionic, both of radius corresponding to 1·32 Å and both octahedral.

A number of pre-assembled model units have been designed, mainly as an aid to building polypeptides and amino-acids. Their purpose is simply to speed up the construction. They are made from the standard atom models and can be taken apart if desired.

D. *Godfrey models*

The Godfrey models (Godfrey, 1959) are made of pliable P.V.C., the colour being incorporated. They are hollow, flexible and compressible. It is claimed that all organic systems can be constructed as a result of the compressibility, including strained rings, and that for this reason only a limited number of models of a particular element are necessary. The area round the bond receptacles in the atom models has been thickened so as to reduce wear and tear. The models are of the Stuart type and in contact when linked. Since, however, the tetrahedral models of carbon and nitrogen are spherical, these must represent only the covalent radii, and there is no indication of the van der Waals's envelope. There are two other carbon models. One is capsule-shaped and has 3 bond receptacles in a planar arrangement about its centre; it is used for both olefins and aromatic rings. The other is disc-shaped and has two bond receptacles in the centre on each side; this is the triple-bond carbon. The atom models become distorted with use but, according to the manufacturers, the original shape can be restored by immersion in boiling water for a few minutes. The writer attempted to remove a dent from a carbonyl–oxygen in this way but found that, although the model was a much better shape afterwards, its radius had decreased by about 2 mm.

Hydrogen bonds are simulated by cutting a slit in the oxygen or nitrogen donor and inserting a small magnet. This is attracted to an iron or steel drawing pin (or another magnet) which is pushed into the rounded surface of the hydrogen model (Figure 8.2*c*).

The connectors are made of polyethylene strips. There are four sizes. The shortest ($\sim$ 1·25 cm) is used for all atom models with more than one bond receptacle, except in the construction of ring systems involving trigonal carbon models when $\frac{1}{2}$ in lengths of plastic rod are used. The connector has a flattened barb at either end with a short neck in between. The other connectors have only one end barbed, and the other end is inserted into the monovalent atom models. These connectors are for use with hydrogen, carbonyl–oxygen and chlorine models. The lengths are $\sim$ 2·65, 4·05 and 5·10 cm, respectively. The lengths of similar connectors vary by up to 1 mm. These are inserted into the model until the surface is touched on the inside. The barbed end then protrudes and may be fitted into another atom model. In the original paper by Godfrey (1959) the use of coiled springs was recommended for large assemblies. These, however, are not supplied in the set sold by Bronwill Scientific Division. Additional stability of the assembled model may be achieved by inserting metal staples into the ends of two adjacent atom models, e.g. the trigonal carbon ones in an aromatic ring.

These models, of moderate accuracy, can serve to represent a number of simple molecules and might be useful for introductory teaching.

E. *Leybold models*

The Leybold models are derived from those designed by Stuart (1952) and Briegleb (1950, 1955). The atom models are made of wood and painted, except for the new hydrogen models which are made of white plastic. When joined they are in contact, and the link makes no contribution to the interatomic distance. Some bonding faces are painted a different colour from the rest of the atom in order to distinguish them. For example, the carbon atom models used in the construction of 5-membered rings have yellow surfaces which should face one another. Where multiple bonding is possible, the models have slits which are aligned in adjacent atoms and into which clamping springs can be inserted; thus rotation about the link is prevented. A double carbon model is used for the two common atoms in fused rings. Models are available as units representing, for example, a carbon 3- and 4-membered ring, allene, epoxide and nitro groups. Bridging atoms enable quite complex ring systems to be constructed. For instance, there is a carbon bridge model for chelate 6-membered rings, as in haemin, and nitrogen bridges for fused 6- and 5-membered rings. The two base pairs adenine–thymine and cytosine–guanine can each be obtained as complete units, greatly facilitating the construction of a DNA model. Metal complexes of various kinds can be constructed using the planar or octahedral covalent or ionic metal models. In addition, there is a planar trivalent aluminium model and a 'siloxane' oxygen with a 132° bond angle. The latter can be used for silicones and related structures and also for 6-membered chelate rings. The hydrogen-bond model is flatter than that of covalent hydrogen, although both contain permanent connectors on the plane faces. The rounded surface of the former has a metal hook attached to it while the corresponding surface of the carbonyl–oxygen atom has a slot which is spanned by a metal staple; the hook is slipped into it and held by the staple (FIGURE 8.2*d*). This 'hook and eye' mechanism is very satisfactory. It is easy to operate, and there is no risk of the 'hydrogen-bonded' models falling apart. The only objection is that the orientation cannot be altered to any significant extent.

The Leybold connectors are strong metal press-studs which are quite easy to manipulate using the separator tool. There is very little friction to prevent rotation about single bonds, and it could be difficult with large assemblies to maintain the required orientation. One end of the separator tool is used to insert and extract the connecting studs; they can, however, usually be inserted with the fingers. The other end of the tool is a levering blade used to separate the models.

The Leybold models provide a large range of structures and, like the Courtauld and C.P.K. ones, are particularly suited to the construction of biochemically important species. However, a great many simpler

organic molecules can be represented and principles such as structural and optical isomerism, tautomerism, mesomerism and chelation readily be demonstrated.

To conclude this Section, a brief account is given of two further examples of space-filling models. The first, known as the Lande–Edmund Molecular Model Kit, is designed for the construction of peptides and proteins and consists of pre-grouped clusters of atom models which represent groups such as indole, imidazole, phenyl, guanido, etc. The models are made of white plastic and joined by pin-type connectors. Free or restricted rotation is possible.

S.A.S.M. models are unusual in that, if short connectors are used, the resulting assembly is of the space-filling kind, but long links (in 6 different lengths proportional to the most commonly occurring bond lengths) are also available, permitting the construction of exploded models in which the scale of the atom models differs from that used for the internuclear distances. These models themselves are of the usual Stuart kind, and a fair range of species is manufactured. There are three scales (1 Å ≡ 1, 1·5 or 2 cm) for the atom models and likewise for the connectors (1 Å ≡ 1, 5 or 10 cm). These are of metal, except for building strained structures for which flexible plastic links are provided, those for space-filling assemblies being dumb-bell-shaped so as to strengthen the link. S.A.S.M. models can be used to construct 'mixed' assemblies in which, for example, an exploded model of an aromatic ring system has space-filling substituents. It is claimed that this type of assembly is useful for teaching purposes because it corresponds more closely to graphic representations of structures than do the space-filling models. For multiple bonding, more than one connector is used.

3 BALL AND SPOKE MODELS

Models of the ball and spoke type are widely used by crystallographers, mineralogists and solid-state physicists as well as by chemists. They can be used to represent every kind of crystal structure and discrete molecule. All types of bonding can be demonstrated. The most accurate models have internuclear distances proportional to the sums of the van der Waals's, covalent or ionic radii of the component atoms or ions, while the least accurate have spokes all the same length. Generally, the spheres are the same size, but a few models have them of different sizes corresponding approximately to the relative ones of the atoms or ions. A large range of crystal-structure models may be bought already assembled, while sets of components are also available. These can play an important part in the teaching of chemistry, even at a very early stage, and have some application to research problems.

Models illustrating close packing are also included in this Section, although some of them show the spheres in contact while others are of the

usual ball and spoke type. There is some justification for this in that the close-packed spheres are usually threaded on to vertical spokes and, since they are also representing essentially ionic structures, they have rather more in common with many of the ball and spoke structures than with the molecular space-filling variety.

A great many phenomena can be demonstrated by the use of ball and spoke models. In some respects, these are similar to those shown by space-filling models, although the two types should be regarded as complementary to each other rather than in competition. Both can be

TABLE 4. BALL AND SPOKE MODELS: CLASSIFICATION OF PRE-ASSEMBLED STRUCTURES

Structural class	*Examples selected from*	
	C.S.L. range	*Leybold range*
1. Crystal systems and elements of symmetry	Bravais lattices, face- and body-centred cubic, hexagonal close-packed, Miller indices	set of crystal systems, Bravais lattices
2. Inorganic structures	NaCl, CsCl, zinc blende, wurtzite, CaF_2, CdI_2, $CdCl_2$, Al_2O_3, $CrCl_3$, Cu_2O, ice (2 forms), ilmenite, La_2O_3, $PbCl_2$, PbO, NiAs, rutile, perovskite, spinel (normal and inverse)	NaCl, CsCl, zinc blende, wurtzite, CaF_2, CdI_2, $CdCl_2$, Al_2O_3, Cu_2O, ice I, PbO, NiAs, rutile, perovskite, spinel
3. Metals and alloys	Al, Ca, Cu, α-, β-, γ-Fe, Hg, Mg, Mn, Na, Sn (grey and white) W, Zn; AuCu, γ-brass, Cu_3Au	Cu, Mg, Sn, U, W; austenite, martensite
4. Silica and silicates	12 silicic acid radicles, quartz, cristobalite, tridymite; beryl, chrysotile, faujasite, mica, vermiculite	quartz, cristobalite, tridymite; topaz, zircon, beryl, diopside, kaolinite; also set of 6 partial silicate models
5. Biochemical structures	α-helix, set of 20 amino-acids; chlorophyll, cholesterol, collagen, DNA, insulin, penicillin	protein α- and γ-spiral
6. Random and defect structures, semiconductors, etc.	Ag_2S, CuO, Ge (*n*- and *p*-type), MnO (magnetic domains shown), several ferrites, edge and screw dislocations	

used to illustrate isomerism, but the more open arrangement in the ball and spoke models enables the differences between isomers to be seen more clearly. The space-filling models are greatly superior in indicating steric hindrance, but it can often be inferred in the ball and spoke type by measuring the distances between non-bonded atoms and scaling down to atomic dimensions. Both kinds can be used to demonstrate reaction mechanisms but, here again, the space-filling models are superior in that the severe steric hindrance often visible in the transition state will indicate the likely outcome of the reaction while this would not

necessarily be apparent in the other type. On the other hand, the design of the ball and spoke models enables relative bond lengths and angles to be seen much more easily.

The great advantage of ball and spoke models lies in their portrayal of crystal structures, and a correlation between structure and properties is often possible. Elements of symmetry are readily demonstrated and crystallographic planes easily identified because of the openness of the structure. In ionic models, the co-ordination number of each ion is quite obvious, whereas in space-filling models it is often difficult to determine the number of nearest neighbours. Polymorphs and allotropes may be distinguished without difficulty even in cases such as α- and β-quartz (FIGURE 8.3) which are structurally very similar. Ball and

TABLE 5. BALL AND SPOKE MODEL COMPONENTS

	C.S.L. wooden spheres and slit spokes	C.S.L. Linnell	Gallenkamp	Griffin & George
No. of different types of sphere (approx.)	19	9	17 (incl. Nuffield Trials components)	20
Types of spoke	slit ends; 23 lengths represent 23 bond lengths; colour-coded; swivel centre spoke for free rotation; non-rotating and two flexible spokes	flexible springs, 1 and 1·5 in	flexible springs, 1, 1·5, 2·4 in	flexible springs, 1·88 and 3·25 in; rigid spokes, 'expendable' wood connectors
Drilling of spheres and symmetry	26-hole, multipurpose 12-hole, close-packing 8-hole, cubic 6-hole, octahedral 5-hole, trig. bi-pyramid 4-hole, tetrahedral 3-hole, planar 2-hole, linear 1-hole	14-hole, multipurpose 5-hole, trig. pyramid 4-hole, tetrahedr. 2-hole, tetrahedr. angle 1-hole	14-hole, multipurpose 8-hole, cubic 6-hole, octahedr. 5-hole, trig. bi-pyramid 4-hole, tetrahedr. 2-hole, tetrahedr. angle 1-hole	8-hole, cubic 6-hole, octahedr. 6-hole, trig. prism 5-hole, trig. bi-pyramid 4-hole, tetrahedr. 2-hole, tetrahedr. angle 1-hole
Colour code	Institute of Physics			Physical Society (halogen yellow)
Scale	5 or 10 cm ≡ 1 Å	~3·5 cm ≡ 1 Å	~3·5 cm ≡ 1 Å	—

spoke models may also be used for random structures and to show various defects such as edge and screw dislocations, non-stoichiometry and semi-conductivity.

A fairly recent commercial development is the flexible spoke. By using two or three of these to form double or triple bonds, multiple bonding appears to reduce the bond length and, in the case of the triple bond, some indication of the symmetry of the electron density about the bond is given. A further advantage is that in highly strained structures the spokes bend and the strain is immediately apparent. The flexibility of the linking mechanism also enables vibrational modes to be demonstrated.

The representation of an ionic crystal by a number of small spheres (often the same size), a considerable distance apart, joined by metal rods, has obvious disadvantages from a theoretical point of view, and these need to be made explicit to students. A slightly less obvious misconception is that stationary ions occupy fixed positions in a perfect crystal. A course on crystal defects appears to be a suitable antidote.

As with the space-filling models, and for the same reason, a few examples of ball and spoke models have been selected for detailed description and as much as possible of the data summarized in TABLES 4 and 5.

A. *Pre-assembled models*

Of the models which can be supplied ready-made, those supplied by Crystal Structures Ltd. (C.S.L.) and Leybold are considered below. The crystal-structure-model panel of the x-ray analysis group of the Institute of Physics published recommendations concerning this type of model (Institute of Physics, 1947):

(1) The scale used for internuclear distances should be
  (*a*) 1 cm ≡ 1 Å for small models
  (*b*) 2·5 cm ≡ 1 Å for general purposes
  (*c*) 5 cm ≡ 1 Å for large lecture-hall demonstrations.

(2) Distances should in general be correct to within 0·1 Å.

(3) Materials should be durable and the dimensions should not change with time.

(4) The connecting spokes must be held securely.

(5) The method of colouring should be permanent.

(6) Spheres should not exceed the equivalent of 1 Å diam. and preferably should be smaller. For a scale of 1 Å ≡ 2·5 cm, spheres of 2 cm diam. are suitable.

(7) It is generally more practicable to use spheres of the same size, but if different sizes are used, these should be in the correct sequence though not necessarily to scale.

(8) Providing the model has sufficient mechanical strength, spokes of any material or gauge may be used; they should not bend readily and should be protected against corrosion.

(9) As far as possible, the spokes should only represent 'bonds', except that a unit cell may be outlined.

(10) All models should include at least one unit cell and there should be a sufficient number of adjacent atoms to show the full co-ordination of all the atoms in the cell.

(11) A durably engraved label should be attached to the model giving the name, chemical composition and all other necessary information.

The recommended colour code is given in TABLE 1.

This summary has been given because, although it was intended to be applied particularly to pre-assembled models, a number of manufacturers of ball and spoke components conform to it wherever appropriate. The colour code has even wider application and is generally used for space-filling and skeletal models.

C.S.L. and Leybold models incorporate all the recommendations except that the C.S.L. spheres are of 2·5 cm diam. for a scale of 1 Å ≡ 2·5 cm and that Leybold use a rather different colour code. A much larger range is available from C.S.L. (nearly 400 models were listed in their 1967 catalogue), and they are prepared to consider making up a model to the customer's specification. The Leybold range of about 130 different models includes structure types similar to those of C.S.L. (see TABLE 4).

Although the spheres are all the same size, C.S.L. have devised a technique whereby the van der Waals's radii of atoms may be simulated and the degree of interpenetration (representing polarization effects) shown. Slightly flexible plastic rods, the same colour as the spheres, are inserted into holes distributed over the entire surface. The rods are then cut to length so as to give an overall radius proportional to the van der Waals's; these are known as 'hedgehogs'.

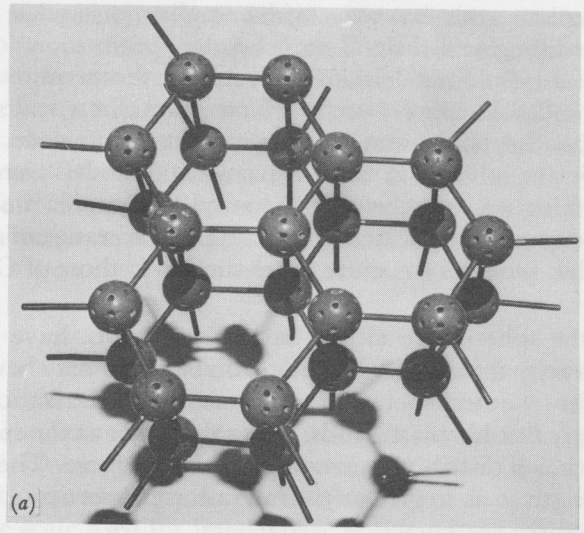
B. *Ball and Spoke Components*

Two different techniques are used in the assembly of these components. The first requires an adjustable base which supports vertical rods on to which the spheres are threaded. Provided that it is possible to change the position of the rods, accurate three-dimensional structures can be built, since vertical spacing may be accomplished by tubular spacers slipped over the rods between the spheres. This method of assembly is used in the construction of the Catalin Ionic and Leybold models (FIGURE 8.4).

The second technique is to drill the spheres in such a way that, when the spokes are inserted into the drilled holes, the common symmetries and valency angles are produced. The final appearance of these models is similar to that of the ready-made structures (FIGURE 8.5).

C. *Models built with an adjustable base*

A very wide range of Catalin Ionic models is available: 36 elements are represented, and there are 41 different ion models; like the Catalin Covalent ones they are of self-coloured plastic. The ion models are made accurately to scale, 1 cm being equivalent to 1 Å. The colours of the ions are related to their positions in the Periodic Table so that, for example, the alkali metals are varying shades of orange. The cations are opaque and the anions transparent; complex ions such as ammonium and hydroxide are mottled. The adjustable base consists of a square plate with side rails along two opposite edges. Attached to the rails and perpendicular to them are a number of cross rails which may be moved



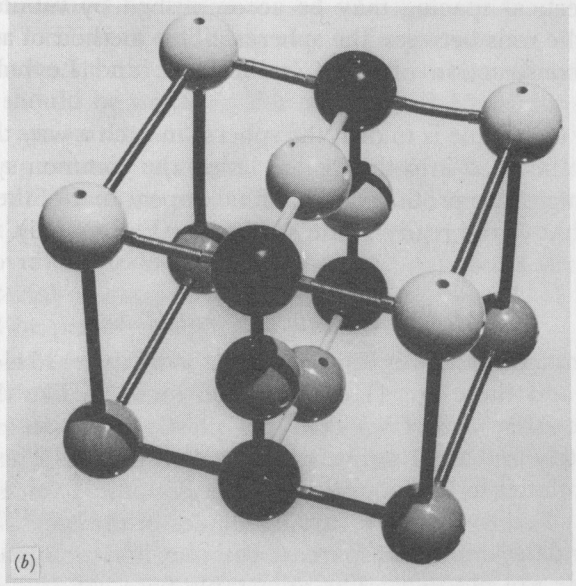


FIGURE 8.5 (continued on opposing page)

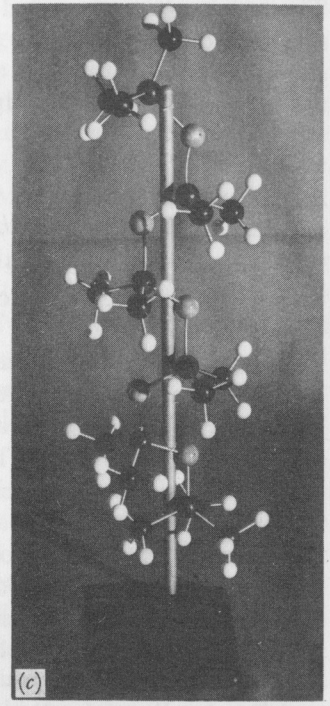


FIGURE 8.5. Models with spoke and drilled sphere components: (*a*) boron nitride (C.S.L.); (*b*) rhenium trioxide (Griffin & George); (*c*) silicone chain (Gallenkamp)

along the former. Vertical rods are fitted into nylon collars on the cross rails, and the rods can be moved along these. The ion models are threaded on to the vertical rods and their position is fixed by polythene sleeving of appropriate length which holds the ion models apart. Thus three-dimensional adjustment of the position of the models is possible. Adjustable bases are available in several different sizes.

A large number of ionic structures can easily be assembled with this technique. It is useful for illustrating close-packed structures, as octahedral and tetrahedral holes are readily identified and their difference in size demonstrated by showing that a small sphere will cause distortion of the lattice if placed in a tetrahedral hole, while an octahedral hole is quite large enough to contain it. Structures can be built so that particular crystal planes are exposed. For example, in a discussion of cubic structures, it is often desirable to be able to show the 111 plane. Since fine adjustment of ion positions is easily brought about, these models can be used to demonstrate dislocations in crystals, disordered structures and various other lattice defects. This type may be used to advantage in the teaching of crystal chemistry at all levels.

The Leybold model has a metal base plate to which the vertical steel rods are attached by magnetic feet. They can, therefore, be placed in any position on the plate, and side and cross rails are unnecessary.

The spheres are threaded on to the vertical rods and separated as required by rubber rings. The spheres are all the same size and there are only three colours. A photograph of a 4-fold screw rotation using the Leybold base appears in Kakabadse and Theobald's paper (1967).

D. *Models with spoke and drilled sphere components*

The examples selected are those supplied by C.S.L., Gallenkamp, and Griffin & George. The accuracy with which these models are scaled varies considerably.

In addition to pre-assembled structures, C.S.L. supply two kinds of ball and spoke components. One, consisting of wooden balls and slit spokes, is the most accurate of the spoke and drilled sphere models selected for discussion. Their standard scale is 5 cm ≡ 1 Å, with 2·5 cm diam. balls, but models can also be built with an overall scale of 10 cm ≡ 1 Å using 5 cm balls and longer spokes. The balls are painted according to the usual colour code. They are drilled so as to be able to represent a number of different symmetries. The 26-hole ball is multipurpose. It can be used to demonstrate 12-co-ordination (in close-packed structures), 8- (cubic and square anti-prism), 6- (octahedral), 5- (trigonal bipyramid), 4- (tetrahedral and square planar), 3- (planar) and 2-co-ordination (linear or tetrahedral angle) quite accurately. Other, less symmetrical, arrangements are also possible but in some cases only approximately. Balls with 12, 8, 6, 5, 4, 3, 2 and 1 holes are also available. To represent van der Waals's radii, either the spare holes in a 26-hole ball can be filled with slightly flexible spokes of suitable length, or 'hedgehogs' can be used.

The spokes used in these models all have slit ends, ensuring a tight fit and minimum wear and tear when inserting or extracting them. There are 23 different spoke lengths in the organic chemistry set, corresponding to 23 different bonds in organic structures. These are colour-coded for easy identification. In addition, there is a spoke with a swivel at the centre which permits rotation. There is also a non-rotating spoke which locks two linked atom models in position. Two kinds of flexible spoke are available. One can be stretched, compressed or bent while the other can only be bent; these can be used for multiple bonds. To bring about minor adjustments in length or angle, a sprung spoke holder can be used. An eyelet is screwed into whichever hole in the sphere represents the best approximation to the correct orientation. The spoke holder is bolted into this and the spoke can then be locked in position after rotating the eyelet so as to obtain the required angle.

The Linnell models (also supplied by C.S.L.) are simpler (and somewhat less accurate). The 2 cm diam. balls are plastic, with 14, 5, 4, 2 or 1 holes, and colour-coded. The 14-hole ball can be used for cubic,

octahedral, tetrahedral, square planar and linear symmetries and, less accurately, for trigonal bipyramidal and trigonal planar arrangements. Some other, less symmetrical, structures can also be assembled.

The spokes are flexible springs in two lengths. The shorter (1 in) are used for all bonds in which hydrogen is joined to another element, the longer (1·5 in) for all others. In this way, an overall scale of very approximately 3·5 cm ≡ 1 Å is obtained. Multiple bonds are formed by using two or three springs as appropriate. Their flexibility enables strained structures to be built with ease. In the construction of aromatic rings, 14-hole balls are joined by double springs. Each is inserted into either the upper or lower hemisphere of each ball, and the result is an interatomic distance intermediate between double and single bond lengths. Although the scale is only approximate, it may be assumed that there will be interaction between non-bonded atoms if they are 7-10 cm apart; this corresponds to 2–3 Å.

The Gallenkamp Linnell models are very similar in design to those of C.S.L.; in fact, the C.S.L. Linnell set and the simplest of the Gallenkamp ones have the same overall approximate scale, colour code and components and differ only in minor detail. However, Gallenkamps also supply two more advanced sets which contain additional components: 'general purpose' 14-hole spheres in two colours (orange and purple), and spokes 2·4 in long. A Gallenkamp Linnell set is being developed for use in schools, for which 8 new atom models have been designed, including 6- and 8-hole sodium and halogen species. The new models will enable a wider range of inorganic structures to be assembled. The Linnell models are quick and easy to assemble and the spokes fit tightly into the spheres, so that there is little risk that they will inadvertently come apart.

The Griffin Skeletal Atomic Models are of the ball and spoke type. There are 8-, 6-, 5-, 4-, 2- and 1-hole balls, with two versions of the 6-hole drilling giving rise to either octahedral or trigonal prism symmetry. Two sizes of sphere (1·25 and 0·75 in diam.) are manufactured but the smaller ones have only two or one holes. The colours used are those recommended by the Colour Group of the Physical Society. The code does not differ markedly from that of the Institute of Physics for the most common elements (which are the only ones represented) except that halogen models are yellow instead of green. However, providing the drillings are appropriate, any code may be used since the models are not intended to be to scale. Flexible springs of 1·88 in or 3·25 in length are used for most purposes but rigid spokes are recommended for large assemblies. For permanent models, or where spokes of a particular length are required, the manufacturers provide 'expendable' wood connectors which may be cut to size and coloured if required.

Data on these and similar models are summarized in Table 5.

4 SKELETAL MODELS

These models, as their name implies, show only the bare framework of molecules and crystal structures. In many respects they are like ball and spoke models, except that the balls are omitted. They vary greatly in precision, complexity and range of application. The most precise are designed primarily to represent covalent structures, particularly those of large organic molecules, and can be used in conjunction with the best space-filling models to which they are complementary. Precise skeletal models are employed extensively in studies of conformational analysis and reaction mechanisms. They consist of metal rods or tubes accurately representing internuclear distances. Plastic or wood tubes or rods, which can easily be cut to size if necessary, are frequently used for the less precise models. These are generally more versatile and serve to build ionic structures, complexes and co-ordination polyhedra as well as organic molecules. Skeletal models have all the advantages of open ones, in that molecular dimensions are clearly seen and bond lengths and angles are accessible and easily measured. However, steric hindrance is less obvious than with ball and spoke types, and space-filling models remain the most suitable for demonstrating this phenomenon. A few skeletal model types are described below.

A. *Dreiding Models*

These are precise, and a large number of organic molecules can be constructed with them (FIGURE 8.6). They consist of stainless steel

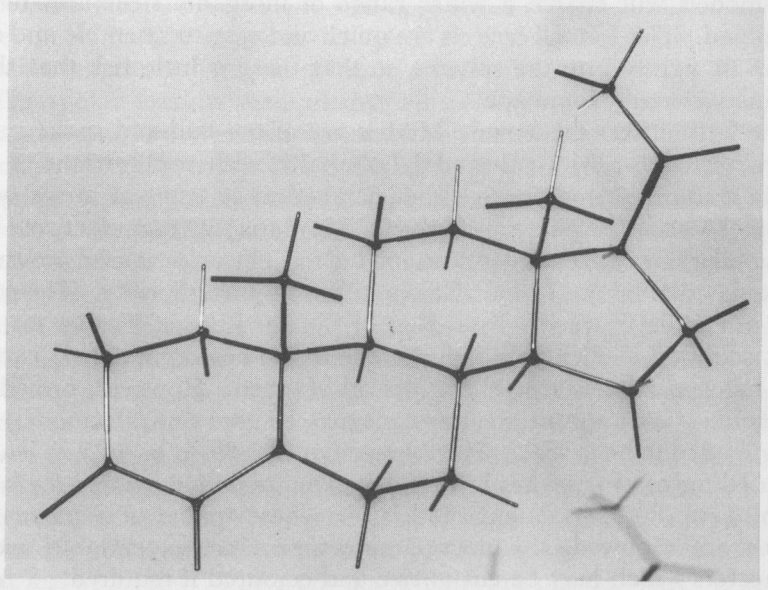


FIGURE 8.6. Dreiding model of progesterone

rods and tubes brazed together in small units representing specific chemical structures. These are joined by inserting the rod of one into the tube of the other until they snap together, indicating that the linking mechanism is holding the units apart at the correct internuclear distance. The link permits free rotation and remains linear and undistorted unless strained. The scale is 1 Å $\equiv$ 2·5 cm, convenient for the assembly of large molecules as the final structure is not too large. The rods and tubes represent σ-bonds only; there is no way of showing π-bonds apart from the shortening of the internuclear distance. The length of each tube or rod in a particular unit represents the distance between the atom at the centre and a hydrogen atom. Thus a methane unit consists of 4 rods or tubes brazed together to give a tetrahedral unit with the length of each proportional to that of a C–H bond. The end of the rod or tube represents the nucleus of the hydrogen atom. If two such units are joined, the new bond will be proportional to the length of the C–C bond. Where rotation about a bond is not possible, the nuclei are brazed together to form a single unit. This technique is used for multiple bonds. Benzene rings, for example, are constructed from three double units. Over 100 different units are listed in the manufacturers' catalogue for 1966. With these it is possible to construct a very large range of cyclic systems, including ring sizes from 3- to 7-membered rings, heterocyclic systems, fused rings, *endo* and *exo* conformations, saturated and unsaturated rings. Moreover, special units can be made to the customer's own specification if required. Use of this service is recommended by the manufacturers if, in the construction of a cyclic compound, the angles are likely to differ by more than a few degrees from the normal value, as otherwise permanent deformation of the units may occur. The different atom nuclei are colour-coded for easy identification and, where ambiguity may arise concerning bond types, these are differentiated by white marker rings; for example, an isolated C=C has one, while a conjugated C=C unit has two. Iron, cobalt and nickel octahedral units are available enabling a number of complexes to be constructed. In addition, there is square planar nickel, tetrahedral tin, lead, zinc, boron, phosphorus and silicon. A B–H–B bridge unit is also provided for the construction of borane models.

Dreiding models are sufficiently precise for accurate measurements to be made. From these, it is possible to estimate the extent of interaction between non-bonded atoms and to evaluate the energy content of different conformations. Alternatively, in some cases the correct conformation can be inferred by comparing the calculated dipole moment of a model with a particular conformation (obtained by vector summation using the Dreiding model) with the observed dipole moment of the molecule. If these agree, it suggests that the model conformation is correct. An experiment of this kind has been done with the boat and chair forms of α-bromocyclohexanone (Kakabadse and Theobald, 1967).

Models similar in design to those of Dreiding but constructed chiefly from plastic material, have been described by Fieser (1963,1965). The basic building unit, essentially similar to that of Dreiding methane, has 4 'bonds' tetrahedrally arranged. Two of these terminate in a short length of preformed aluminium tubing, while the other two consist of plastic rod. In order to keep the cost as low as possible, 'half tetrahedra' are supplied by the manufacturer; the two halves must be cemented or welded together by the purchaser.

The principle of assembly is the same as for the Dreiding models, the extent of insertion of rod into tube being determined by indentations on the latter, thus ensuring correct separation between units, which is proportional to the internuclear distance.

A small number of plastic balls of different size are included in the set. Each has two drillings, one of which can be attached to a rod and the other to a tube. They are used to represent substituents.

The range of components is not as wide as for the Dreiding models, but as the plastic material (Lexan, a polycarbonate) can be readily cut, bent or painted, existing components can easily be modified (Fieser, 1965). The material can be bent through 20°–30° without permanent set, but for the construction of e.g. small ring systems, permanent bending can be brought about after softening with a hot-air blower.

The models are intended primarily for teaching purposes and are not as precise as the Dreiding ones. They are, however, much cheaper and more versatile.

B. *Framework Molecular Models (F.M.M.)*

Although these are less precise than the Dreiding models, they are more versatile and can be used to construct a wide range of structures. They consist of two kinds of component. Firstly, there are three small metal units with 6, 5 or 4 prongs meeting at a common point. These are oriented to represent octahedral, trigonal bipyramidal and tetrahedral arrangements and are copper-, brass- and silver-coloured, respectively. There is also a linear fastener consisting of a tapered rod with a slight projection at the centre, and a 90° angle fastener. The other components are colour-coded plastic tubes which fit over the prongs of the metal units. The octahedral, trigonal bipyramidal and tetrahedral units are called 'valence clusters', and their centres represent those of atoms or ions. There are 12 different colours of solid colour tubing which can be cut to scale as required and used to join like atoms, while two-colour tubing serves for joining unlike atoms. The black and white tube, for example, is approximately 12 cm long and can be cut in half giving two C–H bonds; each consists of a black section corresponding to the covalent radius of carbon, followed by a smaller white section proportional to that of hydrogen. A small black ring represents the hydrogen nucleus, and this is followed by a white section proportional to the van

der Waals's radius of hydrogen. The scale used is 1 Å ≡ 2·5 cm. A similar blue and white tube represents the N–H bond, a red and white one O–H bonds. A somewhat different system is used for C–O and C–N (black/red and black/blue, respectively), as for these only the two covalent radii are represented. The tubes can easily be cut, and their flexibility enables strained rings to be constructed. The trigonal bipyramid 'valence cluster' is used for sp^2 hybrids, the three co-planar prongs for σ-bonds and the two axial ones perpendicular to them to indicate π-bonding. In the ethylene model, two rectangles are constructed above and below the plane of the C–H bonds (and perpendicular to it), between the two carbon atoms; these represent the π-bond. In the acetylene model, octahedral clusters are used and two pairs of rectangles at right angles to each other constructed; these give an indication of cylindrical symmetry about the bond. Similar techniques are employed for other multiple bonds and in all cases result in restricted rotation (Figure 8.7).

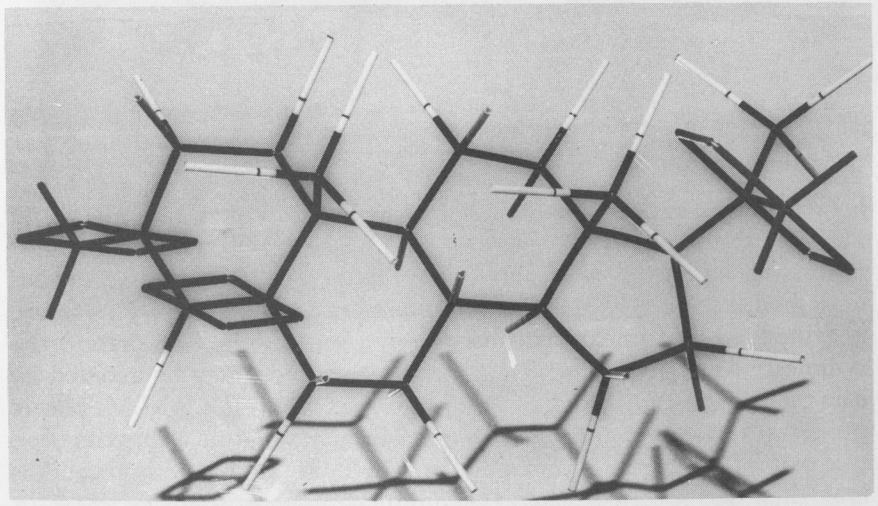


Figure 8.7. F.M.M. model of progesterone

The F.M.M. models are assembled quickly and easily, while the linear connectors may be removed by using pliers. They are cheap, and their versatility makes them extremely useful as a teaching tool, not only for representing many organic compounds but also in inorganic chemistry. Elements of symmetry in a tetrahedron or octahedron can be shown and optical isomerism in metal complexes readily demonstrated. A chelate ring, for example, may be indicated by attaching a long length of tubing to two co-ordination positions in an octahedron so that it bows outwards, thus simulating the usual graphic representation of a chelate ring. The F.M.M. models also provide a quick and easy way

of linking tetrahedra and octahedra to form chains, sheets and three-dimensional arrays such as occur in many inorganic crystals (FIGURE 8.8). The polyhedra are joined by angle fasteners; extra ones can easily

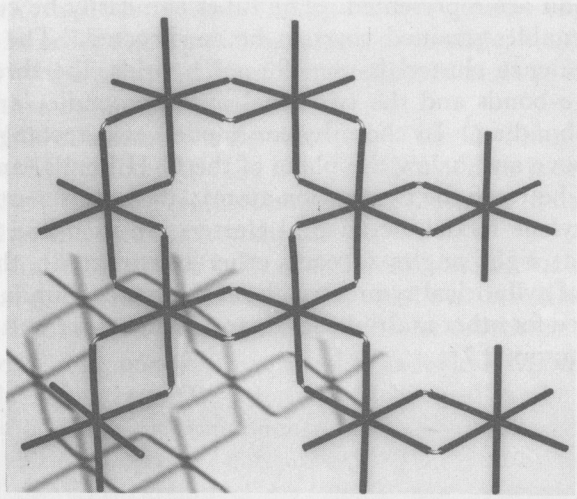


FIGURE 8.8. F.M.M. chromic chloride layer lattice

be made by bending small pieces of wire of suitable gauge at right angles.

A paper by Barrett (1967) describes the use of a new 'valence cluster' in demonstrating $p\pi$–$d\pi$, $d\pi$–$d\pi$ and δ-bonding. A sphere of 1 in diam. is drilled, so that linear fasteners inserted into the holes represent the symmetry axes of the *d* orbitals; however, drilling may be avoided by using a 14-hole Linnell ball. The writer has found the F.M.M. plastic tubes to fit snugly into the holes, and a very reasonable approximation to *d* orbital symmetry is thus obtained. π-Bonding involving *d* orbitals may then be indicated using a technique similar to that described for $p\pi$-bonding.

C. *Geodestix*

These are extremely simple models consisting of plastic rods or tubes, coloured according to length, and soft plastic connectors with 5, 6 or 8 radiating tubes into which the plastic 'sticks' are inserted. There are two kinds of 8-way connector. One has a central hole, the other a through-way joining a pair of opposite connecting tubes; the 5- and 6-way connectors both have central holes. The Geodestix were not designed for modelling to scale, but it is not difficult to devise one (about 5 cm $\equiv$ 1 Å is suitable for many purposes), as the rods are easily cut. The connectors should be eased gently off the rod when dismantling

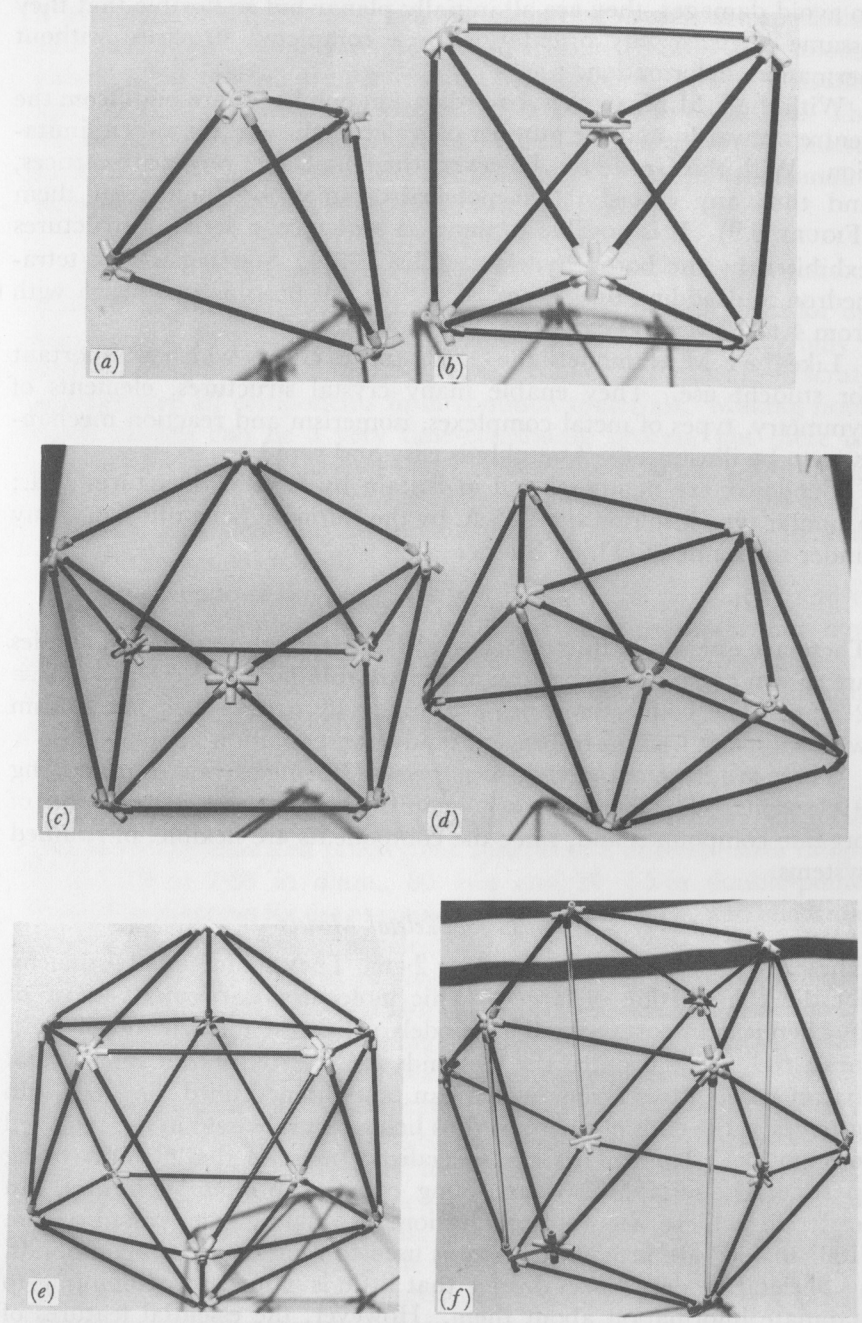


FIGURE 8.9. Co-ordination polyhedra constructed from Geodestix: (*a*) tetrahedron; (*b*) octahedron; (*c*) square antiprism; (*d*) bisdisphenoid; (*e*) icosahedron; (*f*) cubo-octahedron

to avoid damage; they are all initially planar but so flexible that they assume virtually any orientation in a completed structure without permanent deformation.

With the F.M.M. models, co-ordination polyhedra are built from the centre outwards, and the number of 'valence clusters' imposes a limitation. With the Geodestix, however, the connectors represent vertices, and thus any co-ordination polyhedron may be built with them (FIGURE 8.9). It is possible to show, in sequence, a series of structures exhibited by the boron hydrides (Ellis, 1967). Starting with a tetrahedron and adding one 'atom' at a time, all possible polyhedra with from 4 to 12 vertices can easily be demonstrated.

Like the F.M.M. models, the Geodestix are cheap, which is important for student use. They enable many crystal structures, elements of symmetry, types of metal complexes, isomerism and reaction mechanisms to be illustrated. Assembly is easy and rapid.

Geodestix are manufactured in Britain by Crystal Structures Ltd.; a similar type is sold in the U.S.A. by the Edmund Scientific Company under the name of 'Think Sticks'.

D. *Godfrey Stereomodels*

These are essentially framework models. Although tetrahedral species are shown as small spheres, the others are tubular. The scale is 1 Å ≡ 2·5 cm. The connector tubes are joined by a snap-lock mechanism with sufficient friction to prevent inadvertent rotation about bonds.

There are 20 colour-coded atom species (7 being carbon) representing 9 elements. These models are mainly suited to the construction of organic compounds and, since the components are flexible, of strained systems.

E. *Kendrew Skeletal Models*

These are precise; the scale is 1 Å ≡ 2 cm. They are intended primarily for the construction of large organic molecules, particularly those of biochemical importance. The models consist of units made of rigid brass rod. To join units, the two ends are inserted into a small metal barrel bearing two screws which can be tightened until they lock into grooves at the ends of the rods, thus being securely held in the required orientation. The models are specialized, most of the 23 units being particularly suitable for assembling complex protein molecules. In order to achieve accurate orientation, 17 angle gauges ranging from 100° to 130° are provided. Wire is used to represent hydrogen bonds.

Skeletal models are so diverse that little is gained by attempting to tabulate information about them. However, the essential features of the 6 examples given may be briefly summarized. The Dreiding and Kendrew models are precise. Both are designed chiefly for the construction of organic molecules, but while a very large range of units

is available in the Dreiding set, the Kendrew models are specialized and mainly intended for protein structures. The Fieser models, although less precise, are particularly useful because of their versatility and low cost. F.M.M. and Geodestix have many applications. They can be moderately precise or can be used in a general way to illustrate structural principles. The Godfrey models serve to construct small or large organic molecules with reasonable precision.

5 HOME-MADE MODELS AND MISCELLANEOUS DEVICES

With these, the user has to play some part in preparing them for use; how large a part depends on the type. In some cases it may only be necessary to glue spheres together, in others one has to start from scratch and prepare all components from common materials. Making home-made models can be a very time-consuming process, but there is a certain satisfaction in having them 'custom-built' to one's own design. They are also cheap. Their most important advantage, however, is that they may demonstrate some aspects of structure more helpfully than a commercial model.

A brief glance at the literature will indicate the popularity and the diversity of this kind of model, and many more examples may never have been described. The home-made models are classified in a way similar to the manufactured, and a brief account is given of some other devices not otherwise included.

A. *Space-filling models*

Edmund Scientific Co. supply a 'Closed Molecular Model Kit' which comprises 100 moulded polystyrene spheres of 8 different sizes ranging from 0·75 to 2·83 in diam., 80 1-in and 20 1·5-in double-pointed metal dowel screws for use as connectors and 50 each red and black map-marking pins for representing electrons. The spheres have to be coloured by the purchaser and cut to give the appropriate ratio of covalent to van der Waals's radius. It is also necessary, with multivalent atoms, to devise some method of obtaining the correct bond angles (see below).

Griffin Polyzote spheres are available in 6 sizes, from 0·5 to 2 in diam. These, too, are uncoloured but can readily be painted with a gloss paint; they are easily cut. No connectors are supplied, but pipe cleaners or pointed wooden sticks are suitable. Detailed general instructions and a paper-protractor template which may be glued on to card or plywood make the marking out of bonding positions at the correct angle a simple matter. The most suitable scale is 1 Å ≡ 0·5 in.

Apart from these two examples, where spheres are supplied specifically for modelling purposes, spheres of various materials can be obtained from a number of sources. Some of these are given in TABLE 6 (see Appendix); references to others will be found in the literature cited. Tetlow (1964), for example, describes the use of expanded polystyrene

spheres and a specially designed jig for cutting tetrahedral models. Cork spheres were used to represent structures of boron hydrides by Greenwood and Smith (1964), while Farquharson (1964) made papier-mâché models from old copies of *The Times* when other materials were not available; these could be cut to shape after drying in the oven.

A useful apparatus for cutting segments of spheres from slabs of polyurethane foam is described by Doré (1965). Very soft sponge was used, the radii of the spheres being made proportional to the van der Waals's radius of the respective atoms. When the segments were glued together and used to clad a wire-model framework, it was observed that adjacent spheres could be deformed so that the distance between their centres corresponded roughly to the sum of their covalent radii.

Two new space-filling models have recently been made by Homeier and Larsen (1966) from hard-maple spheres; both represent the central metal atom in an 8-co-ordinate complex. One has its connector sockets arranged to give the symmetry of a square antiprism, the other that of a trigonal dodecahedron (bisdisphenoid).

An inexpensive way of obtaining a large number of space-filling models relatively easily is to duplicate existing manufactured models. This technique has been used by Hoover and Shriver (1961) and Kellett and Martin (1966). Moulds are made from latex or silicone rubber using the existing prototype model to shape them. When the mould is cured, epoxy or polyester resin can be poured in and allowed to set. The resin is first coloured with mineral pigment or pharmaceutical dye. After removing the new model from the mould, rough surfaces can be ground smooth, and holes drilled for connector pegs. Instead of resin, surgical plaster may be used which can be painted with water colours preserved by coating the model with plastic spray. Molecular fragments such as half a benzene or cyclohexane ring as well as single atom models may also be made in this way. The two halves of a molecular model are joined with glue when dry. If a suitable manufactured model does not exist, a new prototype can be made from wood and duplicated.

B. *Spherical Models*

Uncut spheres in tangential contact are employed for these models; the sources are mostly the same as for the space-filling ones. Their uses are similar to those described for the Catalin ionic models built on an adjustable base. Much information is provided in a book by Sanderson (1962) which is almost exclusively concerned with models made from spheres in tangential contact. He has devised a system for colouring them so as to denote the electronegativity of the atom represented: highly electronegative atoms are deep blue, and a gradation through green and yellow to red shows increasing electropositivity. In this way,

the polarity in the assembled models is clearly indicated. The size of the atoms is proportional to the covalent and not, as usually, the van der Waals's radius. In addition to the colouring, to each sphere representing an atom, small white spheres are attached according to the number of electrons in the outer shell, and small black ones showing vacancies where electrons might be accommodated. These are in pairs, so that, e.g. one white and one black sphere together indicate a half-filled orbital. To illustrate complex ions, the central sphere has the appropriate number of small magnets attached to it in the correct orientation,

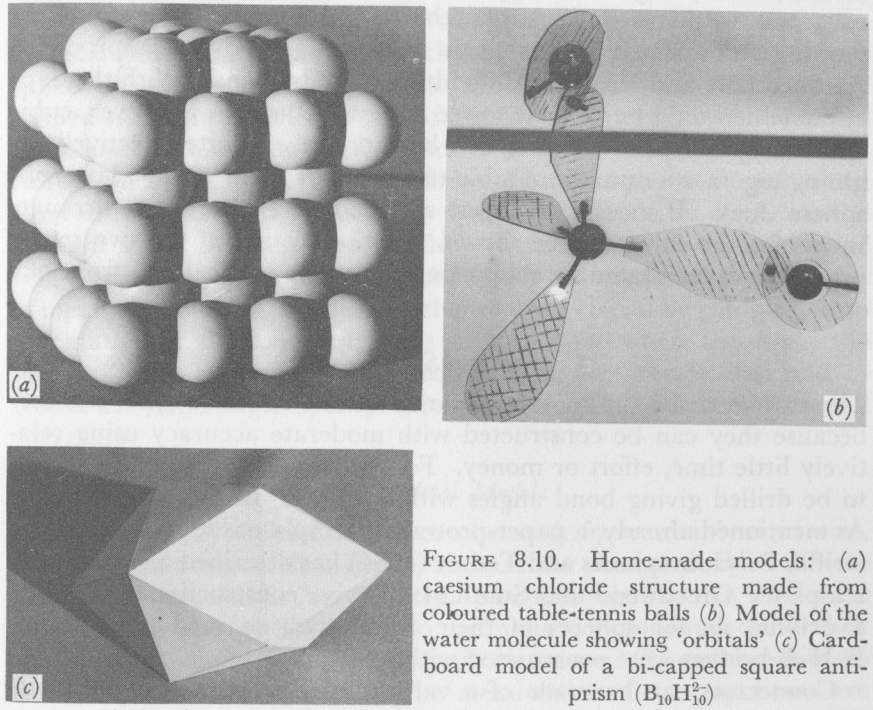


FIGURE 8.10. Home-made models: (*a*) caesium chloride structure made from coloured table-tennis balls (*b*) Model of the water molecule showing 'orbitals' (*c*) Cardboard model of a bi-capped square antiprism ($B_{10}H_{10}^{2-}$)

and in each 'ligand' sphere a small piece of sheet iron is embedded. The larger spheres are usually joined by diamond-shaped wooden connectors in addition to glue so as to improve the mechanical strength of the assembly. Pipe cleaners are suitable for smaller spheres. A great deal of practical information, full details for the assembly of a large number of lattices and a useful bibliography are given.

An interesting technique has been devised for constructing helical molecular models (Tetlow, 1964). The polystyrene spheres are bored, using a hot metal rod, and the back-bone atoms of the chain threaded on to elastic. If the latter is tightened, the tension causes the chain to coil in a helix. The other spheres can then be glued on, using a cheap adhesive made by dissolving polystyrene scraps in benzene.

The process of crystallization in two dimensions can be shown by floating small polystyrene spheres on water (Booth, 1964). If a larger or smaller sphere is included, a 'lattice defect' is observed in the otherwise close-packed formation. The spheres can be hand-made from building board off-cuts which are very cheap. Three-dimensional close-packing can be illustrated by placing spheres in a transparent Perspex cube. Specific planes, e.g. 111, can be coloured and the rest left white.

Coloured table-tennis balls are quite useful for making ionic models, but they tend to be a little more expensive than polystyrene spheres (FIGURE 8.10*a*). Hollow transparent spheres with a small coloured spot on each could well illustrate the two different kinds of close-packing and stacking faults, but do not appear to have been produced commercially and would be difficult to make by hand. With this type of model it would be possible to see *through* the layers. However, cubic and hexagonal close packing can be reproduced quite effectively by gluing together a number of table-tennis balls so as to form a layer one sphere thick. If three such layers are made, the alternative arrangements for the third can be shown. Demonstration of the two sets of interstices is facilitated by supporting the layers vertically in front of a strong light.

C. *Ball and Spoke Models*

These seem to be the most popular of the home-made type, possibly because they can be constructed with moderate accuracy using relatively little time, effort or money. For greater accuracy, spheres have to be drilled giving bond angles within 1° or 2° of the correct value. As mentioned already, a paper-protractor template is supplied with the Griffin Polyzote spheres and Tetlow (1964) has described a home-made template. Greenwood and Smith (1964) give constructional details of a drilling jig for spheres of their boron hydride models; 3-centre B–H–B bridges were constructed with a 90° angle.

Connectors can be made of a variety of materials. Pipe cleaners, wire, orange sticks and wooden cocktail sticks have been used to connect spheres made of polystyrene or similar material which is easily pierced. Another possibility could be coloured plastic cocktail sticks, various colours denoting different bonds. Spheres made of hard rubber or wood, after having been drilled, are usually connected by metal rods or wooden pegs.

Beevers advocates the use of miniature spheres (Kakabadse and Theobald, 1967). He describes a model of sodium chloride in which 1331 small cubes are shown. The coloured Perspex spheres used are in the range 6·6–6·8 mm diam. with an overall scale of 1 cm ≡ 1 Å. The advantages of miniature spheres are the lightness of the models, the ease of storing and their cheapness. Extensive models enable elements of symmetry to be seen more clearly.

A ball and spoke kit is supplied by Edmund Scientific Co., consisting of 50 1-in rubber balls, 50 wooden rods, a sharpener for pointing these and complete directions.

It has been pointed out by Subluskey (1957) that ball and spoke models suffer from the disadvantage that small variations in angle are generally not possible, although it is well known, for example, that 'tetrahedral' angles vary several degrees according to environment. Subluskey has devised a technique whereby variation in angles of this order may be brought about. The spheres are moulded rubber balls, the connector holes being formed during moulding. These have enlarged spherical cavities at the centres of the spheres. The connectors are made from aluminium rod which is turned on a lathe so as to produce spherical enlargements at either end which fit tightly into the similarly shaped holes in the spheres. This fastening mechanism remains secure when under strain. The metal connector can be in two parts, joined by a rubber stock, to allow greater flexibility than the spheres alone permit. Curved rods are used for multiple bonds. Variation in angle can be brought about by stresses due to the structures themselves, as in small ring systems, or with a bond-restraining clip consisting of curved pieces of metal with cut-out sections at either end which can be clamped on to indentations in the connecting rods near the point where they enter the spheres. The curvature of the bond-restraining clip is designed to reduce the bond angle by a specified amount. A jig ensures the correct curvature.

D. *Skeletal Models*

Rough and ready skeletal models can be made from suitably rigid wire, but for accurate models a device such as the Kennard–Doré Stereo-Model Construction Set can be used. Magnetic chucks on a base plate support vertical clamps which hold the model components, so that they can be manoeuvred into the required orientation. Thus three-dimensional adjustment is possible. The metal-rod model components are cut to length with the calibrated cutter supplied and clamped firmly in the correct position while being soldered together. The correct bond angles are obtained by means of one of the 36 plastic angle pieces provided which range from 55° to 125·5°. A pendant clinometer is used for non-planar junctions. The set contains all the necessary equipment including soldering apparatus and an instruction manual.

Harris and Cheung (1962) have used skeletal models made from aluminium tubing to illustrate molecular deformation due to overcrowding, and thus to infer probable transition states in some configurational inversions. The tubing is sawn into appropriate lengths and then lined at the ends with tubular nylon sleeves. The connectors are brass soldering tags, the narrow ends of which are forced into the sleeves. The lengths of tubing, representing bonds, can then be joined by a nut

and bolt using the holes in the soldering tags. Where free rotation about a bond is required, the length of tubing can be sawn in half and a brass rod, covered with a nylon sleeve, inserted into the two halves. This then forms a pivot.

E. *Models Depicting Atomic and Molecular Orbitals*

Sets of orbital models can now be obtained from Crystal Structures Ltd.; there is one complete and two partial ones. The first includes representations of all the *s*, *p*, *d*, and *f* and some *sp* hybrid orbitals. These, with extra *p* orbitals, can be used to demonstrate a wide range of molecular orbitals. The partial sets contain no *f* orbital models and smaller numbers of components. The three-dimensional atomic orbital models illustrate the angular distribution in the *s*, *p*, *d* and *f* orbitals. Different colours are used to indicate whether lobes are positive or negative. The models are attached to a framework of metal rods representing the *x*, *y* and *z* axes which pass through or between the lobes as appropriate. The models, mounted on a cylindrical base, are free-standing and about 10 in high. The sets also contain tetrahedral frames and small white spheres representing point charges which can be used to demonstrate crystal-field effects. The models, designed by Norbury (1968), may be regarded as three-dimensional plots of the angular variation of the wave function: ψ rather than ψ^2 is portrayed. They can be used to illustrate molecular geometry, the effect of ligand fields of different symmetries on the degeneracy of the orbitals and the way in which overlap can occur between metal and ligand orbitals in complexes.

Wire and cork representations of orbitals (for example, with lone pairs of electrons) can be attached to standard molecular models (Kakabadse and Theobald, 1967).

A molecular framework may be made by soldering together pieces of brass or copper welding wire. This can then be clad with plasticine using different colours to represent *s*, *sp*, sp^2, sp^3 or π-orbitals (Vaughan-Williams, 1966).

Two-dimensional representations of orbital shapes can be cut out of Perspex sheet $\frac{1}{16}$ in thick. In these models, designed by Aylett (1958), the atomic nuclei are represented by 26-hole drilled wooden spheres supplied by Crystal Structures Ltd. Slit spokes (also supplied by C.S.L.) are cut in half and the cut end drilled so that it can be bolted on to the orbital shape through similar drilled holes. By using 26-hole spheres, most of the common symmetries can be demonstrated. The model of the water molecule (FIGURE 8.10*b*) shows how the covalent O–H bond is formed by overlap of the *s* hydrogen orbital with the sp^3 hybrid oxygen orbital. The two shapes are drilled and held together by a nut and bolt. Perspex can easily be marked with a grease pencil, suitable markings indicating whether an orbital contains one electron or a pair.

The concept of molecular shape as determined by electron-pair repulsions (Sidgwick and Powell, 1940; Gillespie and Nyholm, 1957) can be illustrated by mechanical analogy using modelling balloons (Jones and Bentley, 1961; Jones, 1965). The theory of electron-pair repulsions assumes that these are greatest for lone-pair–lone-pair, least for bond-pair–bond-pair and intermediate for lone-pair–bond-pair interactions. Also, since a higher electron density is associated with multiple than with single bonds, interactions between two multiple bonds will be greater than those between two single, while multiple-bond–single-bond interactions are intermediate in size. Elongated modelling balloons can be twisted after inflation so that a narrow neck is formed, and two or more can be joined by twisting them together. If two of similar size are so joined at their mid-points and released, the lobes formed point towards the corners of a regular tetrahedron; three balloons form 6 lobes in an octahedral disposition. These symmetrical arrangements are the result of mechanical repulsions between the lobes. To represent an odd number of electron pairs, an extra balloon of suitable size may be twisted in at the junction. Three lobes produce a planar trigonal arrangement, five that of a trigonal bipyramid. To demonstrate double bonds, two lobes, say, of a tetrahedral arrangement are joined with an elastic band so that a trigonal system such as occurs in carbonyl halides results. Two pairs of lobes joined produce a linear structure as in carbon dioxide. Similar treatment of an octahedral arrangement can illustrate the tetrahedral structure of sulphuryl halide molecules (2 pairs joined) or the planar arrangement in sulphur trioxide (3 pairs joined).

Since lone pairs have the largest repulsive effect, these may be represented by short fat balloons, and bond pairs by long thin ones. In this way, a structure representing the water molecule can be made by twisting together two balloons of different sizes, thus forming two short fat lobes with an angle between them greater than, and two long thin lobes with one less than, the tetrahedral. If another thin lobe is twisted into this assembly, the balloons spontaneously arrange themselves with the lobes directed to the corners of a distorted trigonal bipyramid. The three thin lobes are planar, arranged in a distorted T shape. Thus this assembly can represent the chlorine trifluoride molecule.

The modelling balloons can be used to show *cis–trans* isomerism in alkenes. Two long ones of different colours are twisted together at two points, demonstrating one of the isomers. Rotation of the terminal groups at one end will produce the other.

The Walden inversion and S_N2 reactions in octahedral systems can be visualized by tying in an extra uninflated balloon to represent the incoming group, inflating it *in situ* and removing the outgoing one with a pin.

F. *Geometrical Shapes*

Shapes representing the common co-ordination polyhedra can be made from cardboard or stiff paper (FIGURE 8.10*c*). They have been used extensively to build large assemblies consisting of linked tetrahedra or octahedra. The most difficult part of the operation is designing the two-dimensional pattern so that, when it is cut out, folded and the edges glued together, a satisfactory polyhedron is obtained. Diagrams of cut-outs for the icosahedron and various boron-hydride structures are given by Greenwood and Smith (1964), and the Edmund Scientific Co. supply a set of 12 card cut-outs from which most of the common polyhedra can be constructed. Assemblies consisting of linked polyhedra made from wood have also been constructed, but the process is very tedious.

As an alternative, sets of geometric shapes may be bought ready-made. The same company supplies 3 different sets of varying complexity and price.

In Britain, top-quality, precise polyhedra, made of transparent material, can be obtained from Scientific Teaching Apparatus Ltd. However, manufactured sets are often designed primarily for mathematicians, and chemists will hardly find a use for all the components. Moreover, they tend to be rather expensive. It should also be pointed out that models of co-ordination polyhedra can be assembled very easily with Geodestix, as described in the Section on skeletal models (FIGURE 8.9).

G. *Dynamic Models*

While this Chapter is concerned chiefly with static models, some dynamic ones of interest are discussed briefly below.

A series of papers by Kihara (1960, 1963, 1966) describes molecular models which are 'self-crystallizing'. Their purpose is to show that the structures of molecular crystals can arise from interactions between electric multipoles in the molecules. An example cited is that of hexamethylenetetramine. The molecule consists of 4 nitrogen atoms at the corners of a regular tetrahedron which are linked by 6 methylene bridges. The nearly spherical surface of the molecule is composed of 4 regions of negative charge, associated with the nitrogen atoms, and 4 of relatively positive charge in between. It, therefore, corresponds approximately to an octupolar sphere. The model consists of 8 pieces of barium ferrite magnet, 4 of which are magnetized outwards, the others inwards, representing oppositely charged areas on the surface. When a sufficient number of these octupolar spheres is brought together, the resulting assembly represents the true crystal structure of hexamethylenetetramine.

A manually operated model essentially of the ball and spoke type has been designed by Berry and Botterrill (1967) to demonstrate the Walden

TABLE 6. SUPPLIERS OF MODELS AND COMPONENTS

Model or Component	*Supplier*	*Address; approximate price of set*
1. Catalin Covalent Models	Catalin Ltd.	Waltham Abbey, Essex. (£20, £40)
2. Courtauld Models	Griffin & George Ltd.	Ealing Road, Alperton, Wembley, Middx. (£8, £33; Ealing Scientific Ltd. [3a]: sets up to £195)
3. C.P.K. Models	(*a*) Ealing Scientific Ltd.	23, Leman St., London, E.1. (£40–£520)
	(*b*) Schwarz Bioresearch Inc.	Mountain View Ave., Orangeburg, New York, U.S.A. ($90–$230)
4. Godfrey Models	Bronwill Scientific	Box 277, Rochester 1, New York, U.S.A. ($50)
5. Leybold Models	(*a*) E. Leybold's Nachfolger	5 Köln-Bayental, Germany
	(*b*) Scientific Teaching Apparatus Ltd.	Colquhoun House, 27–37, Broadwick St., London, W.1. (£21, £37, £56)
6. S.A.S.M. Models	S.A.S.M.	99 rue Oberkampf, Paris XI^{e}, France. (180–1900 Ffrs)
7. C.S.L. Pre-assembled ball and spoke models	Crystal Structures Ltd.	Bottisham, Cambridge (ind. models, £1–£100)
8. Leybold pre-assembled models	As 5	(£1–£26)
9. Catalin Ionic Models	As 1	(£17, £30)
10. Leybold Crystal Lattice Models	As 5	(£25)
11. C.S.L. ball and spoke components; Linnell models	As 7	(£3–£11; lecture demonstration set, £70)
12. Gallenkamp Linnell Models	Gallenkamp	Technico House, Christopher Street, London, E.C.2. (£3–£25)
13. Griffin Skeletal Atomic Models	As 2	(£10–£17)
14. Dreiding models	(*a*) W. Büchi	Glasapparate-Fabrik, Flawil, Switzerland
	(*b*) Koch-Light Laboratories Ltd.	Colnbrook, Bucks. (£14, £22, £40)
15. Fieser models	Rinco Instruments Co. Inc.	Greenville, Ill., U.S.A. (ca. $5)
16. F.M.M.	(*a*) Prentice-Hall Inc.	Englewood Cliffs, New Jersey, U.S.A.
	(*b*) Prentice-Hall International	Pegasus House, Golden Lane, London, E.C.1. (£2, £59)
17. Geodestix	As 7	(ca. £4)
18. Think-Sticks	Edmund Scientific Company;	Barrington, New Jersey, 08007, U.S.A. ($3–7)
	exporters: Sigma International Inc.	13A, East 40th St., New York, U.S.A. 10016
19. Godfrey Stereomodels	As 4	($30)
20. Kendrew Skeletal Models	As 3*a*	(ca. £30)
21. Edmund Closed Molecular Model Kit	As 18	($12)
22. Griffin Polyzote Spheres	As 2	(ca. £1 per 100)
23. Expanded polystyrene spheres	Elford Plastics Ltd.	Wood St., Elland, Yorks. (12s. to £3 per 100)
24. Styrofoam spheres	Frostee Sno Co.	Depot St., Antioch, Illinois, U.S.A.
25. Polystyrene spheres	Plasteel Corp.	26970 Princeton Inkster, Michigan, U.S.A.
26. Flexocel L. 128 (soft foam)	Baxenden Chemical Co. Ltd.	Clifton House, Euston Road, London, N.W.1
27. Cork spheres	Barthes-Roberts Ltd.	59, Lant St., London, S.E.1
28. Wooden spheres	Wood Components Ltd.	Team Valley Trading Estate, Low Fell, Gateshead, Co. Durham
	W. Purves & Sons	Walkergate, Newcastle-upon-Tyne
29. Ball and spoke kit (rubber spheres)	As 18	($3)
30. Kennard–Doré Stereo-Model Construction Set	As 3*a*	(£145)
31. Set of atomic orbitals	As 7	(£23, £30, £60)
32. Card cut-outs for making geometric shapes	As 18	($1)
33. Manufactured geometric shapes	As 18 and 5*b*	($6, $40, $64)

inversion. An incoming group (–OH) pushes out outgoing group *X* which is situated on the opposite side of the carbon atom. A similar model for demonstrating S_N2 reactions has been designed by Nyquist (1965).

The writer wishes to thank Mr. Derek Taylor of Griffin & George Ltd. for the loan of several sets of models and for his valuable advice and assistance. She also expresses her gratitude to her colleagues of the Chemistry Department, Westfield College, for their co-operation.

APPENDIX: SUPPLIERS AND PRICES

Manufacturers and suppliers of models are listed in TABLE 6. Approximate prices of sets, or estimated cost of usable numbers of components, are given; these should be regarded merely as a guide to the order of outlay involved.

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